> $M_{H2} := 2.016; M_{O2} := 32; M_{N2} := 28.02; M_{H2O} := 18.016; M_{OH} := 17.008; R := 8314; Tref := 295; pref := 101325; p0 := pref;$

R is in J/kmol*K.

> $YH2_1 := 1; YH2O_2 := 0.0072; YO2_2 := (1 - YH2O_2)\frac{M_{O2}}{M_{O2} + 3.76\, M_{N2}}; YN2_2 := (1 - YH2O_2)\, \frac{3.76\, M_{N2}}{M_{O2} + 3.76\, M_{N2}}; QH2 := 119950e3;$

SANDIA H2 − flame undiluted. $H2 + 0.5(O2 + 3.76\,N2) \rightarrow H2O + 1.88\,N2$.

> $r_f := \frac{0.5(M_{O2} + 3.76\, M_{N2})}{M_{H2}}; rho1 := 0.081; rho2 := 1.2; T2 := 294; T1 := 295;$
#Fuel exit temperature is 295K (±2K), the ambient temperature is 294K (±2K)

The turbulent Schmidt and Prandtl numbers are approxiamately 0.7 for an unconfined turbulent jet. The stoichiometric mixture fraction is calculated from the assumption that

$$\left(Y_{fu} - \frac{1}{r_f} Y_{ox}\right) = 0 \text{ when } \xi = \xi_{st}.\ \xi_{st} = \left(1 + \frac{r_f (Y_{fu})_1}{(Y_{ox})_2}\right)^{-1} = \frac{1}{r_f + 1}.$$

> $\xi_{st} := \frac{1}{1 + r_f}; d := 3.75; L := 180 \cdot d;$
$Sc_t := 0.7; Pr_t := 0.7$;*#The diameter is given in mm*

> $pos := Matrix(1..7, 1..14); chementropy := Matrix(1..7, 1..14); heatentropy := Matrix(1..7, 1..14); massentropy := Matrix(1..7, 1..14);$

all the data points are stored in an m x n array, where m is the position along the length of the flame, while n is the axial coordinate.

> $pos := \langle 0, 2, 4, 6, 8, 10, 12, 14, 16, 18, 0, 0, 0, 0;$
$0, 3, 6, 9, 12, 15, 18, 21, 24, 27, 30, 0, 0, 0;$
$0, 4, 8, 12, 16, 20, 24, 28, 32, 36, 40, 44, 48, 0;$
$0, 4, 8, 12, 16, 20, 24, 28, 32, 36, 40, 48, 56, 0;$
$0, 4, 8, 12, 16, 20, 24, 28, 32, 36, 40, 44, 48, 52;$
$0, 5, 10, 15, 20, 25, 30, 35, 40, 45, 55, 0, 0, 0;$
$0, 5, 10, 20, 30, 40, 50, 0, 0, 0, 0, 0, 0, 0\rangle$

> $axial := \left\langle \frac{1}{8}, \frac{1}{4}, \frac{3}{8}, \frac{1}{2}, \frac{5}{8}, \frac{3}{4}, 1 \right\rangle; \xi_{max} := \langle 0.2607, 0.1082, 0.0711, 0.0515, 0.0348, 0.0252, 0.0128\rangle; \xi_{min} := \langle 0.0009, 0.0034, 0.0021, 0.0025, 0.0054, 0.0047, 0.0049\rangle;$
#axial is the distance from the outlet divided by the length of the flame with index m

> $\lambda_{H2} := 3.2778e\text{-}008\, T^2 + 0.00032748\, T + 0.090588; \lambda_{N2} := 5.3835e\text{-}005\, T + 0.011313; \lambda_{O2} := 6.0545e\text{-}005\, T + 0.0097264; \lambda_{H2O} := 1.3815e\text{-}008\, T^2 + 6.635e\text{-}005\, T - 0.0026736;$
#Curvefits of the conductivity of each species

>

Curvefits of thermodynamic properties are found from "The Chemkin Thermodynamic Database", by Sandia. The values "a" are for 300-1000K and the values "b" are 1000-5000K. Note that H°(T) = H°(T)

- H°(298) + Hf°(298), where Hf°(298) is the species heat of formation at 298K, H°(T) is the standard enthalpy at temperature T, and H°(298) is the standard enthalpy at 298K.

```
> thermoprop :=proc(k)local a1, a2, a3, a4, a5, a6, a7, b1, b2, b3, b4, b5, b6, b7;

  if k = H2 then
  a1 := 0.03298124e2;
  a2 := 0.0829441e−2;
  a3 :=-0.08143015e−5;
  a4 :=-0.09475434e−9;
  a5 := 0.04134872e−11;
  a6 :=-0.10125209e4;
  a7 :=-0.03294094e2;
  b1 := 0.02991423e2;
  b2 := 0.07000644e-2;
  b3 :=-0.05633828e−6;
  b4 :=-0.09231578e−10;
  b5 := 0.15827519e−14;
  b6 :=-0.08350340e4;
  b7 :=-0.03294094e2;
  elif k = O2 then
  a1 := 0.03212936e2;
  a2 := 0.11274864e−2;
  a3 :=-0.05756150e−5;
  a4 := 0.13138773e−8;
  a5 :=-0.08768554e−11;
  a6 :=-0.10052490e4;
  a7 := 0.06034737e2;
  b1 := 0.036697578e2;
  b2 := 0.06135197e−2;
  b3 :=-0.12588420e−6;
  b4 := 0.01775281e−9;
  b5 :=-0.11364354e−14;
  b6 :=-0.12339301e4;
  b7 := 0.03189165e2;
  elif k = N2 then
  a1 := 0.03298677e2;
  a2 := 0.14082404e−2;
  a3 :=-0.03963222e−4;
  a4 := 0.05641515e−7;
  a5 :=-0.02444854e−10;
  a6 :=-0.10208999e4;
  a7 := 0.03950372e2;
  b1 := 0.02926640e2;
  b2 := 0.14879768e−2;
  b3 :=-0.05684760e−5;
  b4 := 0.10097038e−9;
  b5 :=-0.06753351e−13;
  b6 :=-0.09227977e4;
  b7 := 0.05980528e2;
  elif k = H2O then
  a1 := 0.03386842e2;
  a2 := 0.03474982e−1;
```

$a3 := -0.06354696e-4;$
$a4 := 0.06968581e-7;$
$a5 := -0.02506588e-10;$
$a6 := -0.03020811e6;$
$a7 := 0.02590232e2;$
$b1 := 0.02672145e2;$
$b2 := 0.03056293e-1;$
$b3 := -0.08730260e-5;$
$b4 := 0.12009964e-9;$
$b5 := -0.06391618e-13;$
$b6 := -0.02989921e6;$
$b7 := 0.06862817e2;$
else
print(*Invalid species*);

end if;

$$cplow_k := \frac{R}{M_k}\left(a1 + a2 \cdot T + a3 \cdot T^2 + a4 \cdot T^3 + a5 \cdot T^4\right);$$

$$cphigh_k := \frac{R}{M_k}\left(b1 + b2 \cdot T + b3 \cdot T^2 + b4 \cdot T^3 + b5 \cdot T^4\right);$$

$$hlow_k := \frac{R \cdot T}{M_k}\left(a1 + \frac{a2}{2} \cdot T + \frac{a3}{3} \cdot T^2 + \frac{a4}{4} \cdot T^3 + \frac{a5}{5} \cdot T^4 + \frac{a6}{T}\right);$$

$$hhigh_k := \frac{R \cdot T}{M_k}\left(b1 + \frac{b2}{2} \cdot T + \frac{b3}{3} \cdot T^2 + \frac{b4}{4} \cdot T^3 + \frac{b5}{5} \cdot T^4 + \frac{b6}{T}\right);$$

$$slow_k := \frac{R}{M_k}\left(a1 \cdot \ln(T) + a2 \cdot T + \frac{a3}{2} \cdot T^2 + \frac{a4}{3} \cdot T^3 + \frac{a5}{4} \cdot T^4 + a7\right);$$

$$shigh_k := \frac{R}{M_k}\left(b1 \cdot \ln(T) + b2 \cdot T + \frac{b3}{2} \cdot T^2 + \frac{b4}{3} \cdot T^3 + \frac{b5}{4} \cdot T^4 + b7\right);$$

return $cplow_k, cphigh_k, hlow_k, hhigh_k, slow_k, shigh_k$
end proc;

```
>
> with(Student[NumericalAnalysis]);
```

Calculate the probability distribution with a beta function.

> $f :=$ **proc**(*xiav* , *xivar*) **local** a, b, B; $a := -\dfrac{xiav\,(xivar - xiav \cdot (1 - xiav))}{xivar}$; $b := \dfrac{(xiav - 1)\,(xivar - xiav \cdot (1 - xiav))}{xivar}$;

if $a > 0$ **and** $b > 0$ **then**

$$B := \frac{\mathrm{GAMMA}(a) \cdot \mathrm{GAMMA}(b)}{\mathrm{GAMMA}(a + b)};$$

xi^(a-1) * (1-xi)^(b-1) / B;
else

```
0;
end if;
end proc;
```

m is the index of the vector axial[] which describes the distance from the fuel outlet

```
> m := 7;
```

The chemical potential is the same as the gibbs function or h-Ts.

```
> μ :=proc(Species) local k;
 if Species = H2 or Species = N2 or Species = O2 or Species = H2O
then k := Species;
else print(Invalid input);
 end if;

cplow[k], cphigh[k], hlow[k], hhigh[k], slow[k], shigh[k] := thermoprop(k);
 h[k] := piecewise(300 ≤ T and T ≤ 1000, hlow[k], 1000 < T and T ≤ 5000, hhigh[k]);
 if ξ_max(m) > ξ_st then
 s[k] := piecewise(300 ≤ T and T ≤ 1000, slow[k], 1000 < T and T ≤ 5000, shigh[k])
      - R/M[k] ln(p[k]/pref);
 else
 s[k] := piecewise(300 ≤ T and T ≤ 1000, slow[k], 1000 < T and T ≤ 5000, shigh[k]);
 end if;
 h[k] - Tref·s[k];
end proc; #Output is Gibbs energy per kg
> for k in [H2, O2, N2, H2O] do potTp[k] := mu(k); end do
> for k in [H2, O2, N2, H2O] do cplow[k], cphigh[k], dummy1, dummy2, dummy3, dummy4
      := thermoprop(k); cp[k] := piecewise(T < 1000, cplow[k], T ≥ 1000 and T ≤ 5000,
      cphigh[k]); end do;
>
>
```

This part assigns the respective curve fits for each segment of the flame

```
> if axial(m) = 1/8 then
 T := 2.2845e+009 xi^7 - 2.2908e+009 xi^6 + 9.3662e+008 xi^5 - 2.0293e+008 xi^4
      + 2.561e+007 xi^3 - 1.9559e+006 xi^2 + 82352 xi + 325.71;
  meanxi := -6.7271e-6 r^4 + 0.0003342 r^3 - 0.0048093 r^2 + 0.00319 r + 0.26057;
  varxi := -8.259e-008 r^5 + 3.8827e-006 r^4 - 6.054e-005 r^3 + 0.00031975 r^2
      - 0.00026386 r + 0.002692;
 radxi := -5.3149e-006 r^4 + 0.0003024 r^3 - 0.0047274 r^2 + 0.0037544 r + 0.2603;
 Y[H2] := 43.961 xi^4 - 30.746 xi^3 + 7.6998 xi^2 + 0.24988 xi - 0.00063242;
 Y[O2] := 354.47 xi^4 - 249.22 xi^3 + 62.403 xi^2 - 6.2713 xi + 0.22559;
 Y[N2] := -0.98592 xi + 0.75955;
 Y[H2O] := -397.12 xi^4 + 274.39 xi^3 - 68.021 xi^2 + 6.813 xi + 0.015694;
 Y[OH] := 202.37 xi^5 - 157.11 xi^4 + 45.137 xi^3 - 5.71 xi^2 + 0.27257 xi - 0.00022817;
 X[H2] := -8.7529 xi^2 + 5.397 xi - 0.022857;
```

$X_{O2} := -1441\ xi^5 + 1283.3\ xi^4 - 447.85\ xi^3 + 76.318\ xi^2 - 6.2783\ xi + 0.20293;$

$X_{N2} := -29.111\ xi^3 + 21.358\ xi^2 - 6.107\ xi + 0.77909;$

$X_{H2O} := -696.42\ xi^4 + 455.5\ xi^3 - 102.05\ xi^2 + 8.1434\ xi + 0.029743;$

$u := -3.2204e\text{-}8\ r^6 + 1.5829e\text{-}8\ r^5 + 1.1141e\text{-}4\ r^4 - 2.0003e\text{-}5\ r^3 - 0.12112\ r^2 + 0.0028871\ r + 42.628;$

elif $axial(m) = \frac{1}{4}$ **then**

$T := -3.6215e7\ xi^4 + 1.2448e7\ xi^3 - 1.6084e6\ xi^2 + 84845\ xi + 325.98;$

$meanxi := 7.1858e\text{-}006\ r^3 - 0.0003255\ r^2 - 5.9972e\text{-}005\ r + 0.10907;$

$varxi := -6.4692e\text{-}011\ r^6 + 5.8962e\text{-}009\ r^5 - 1.9805e\text{-}007\ r^4 + 3.0079e\text{-}006\ r^3 - 2.1417e\text{-}005\ r^2 + 5.8457e\text{-}005\ r + 0.0006821;$

$radxi := 9.5866e\text{-}6\ r^3 - 0.00042613\ r^2 + 0.00068464\ r + 0.10822;$

$Y_{H2} := 249.54\ xi^4 - 92.929\ xi^3 + 14.41\ xi^2 - 0.013771\ xi - 3.0224e\text{-}5;$

$Y_{O2} := 2072.3\ xi^4 - 769.87\ xi^3 + 117.88\ xi^2 - 8.397\ xi + 0.2309;$

$Y_{N2} := -38.207\ xi^3 + 4.6597\ xi^2 - 1.0334\ xi + 0.76424;$

$Y_{H2O} := -1560.5\ xi^4 + 705.88\ xi^3 - 120.08\ xi^2 + 8.9282\ xi + 0.0062749;$

$Y_{OH} := -4870.5\ xi^5 + 1257\ xi^4 - 92.204\ xi^3 + 0.015992\ xi^2 + 0.15694\ xi - 0.00032783;$

$X_{H2} := 3306.9\ xi^4 - 1180.4\ xi^3 + 130.6\ xi^2 + 0.22705\ xi - 0.001419;$

$X_{O2} := 2161.5\ xi^4 - 790.57\ xi^3 + 115.07\ xi^2 - 7.7892\ xi + 0.20551;$

$X_{N2} := -1274.5\ xi^4 + 348.53\ xi^3 - 15.177\ xi^2 - 5.2214\ xi + 0.78292;$

$X_{H2O} := -3951.1\ xi^4 + 1537.4\ xi^3 - 220.79\ xi^2 + 12.406\ xi + 0.014185;$

$u := -3.2204e\text{-}8\ r^6 + 1.5829e\text{-}8\ r^5 + 1.1141e\text{-}4\ r^4 - 2.0003e\text{-}5\ r^3 - 0.12112\ r^2 + 0.0028871\ r + 42.628;$

elif $axial(m) = \frac{3}{8}$ **then**

$T := 7.8498e{+}006\ xi^3 - 1.5371e{+}006\ xi^2 + 91656\ xi + 288.22;$

$meanxi := -3.4567e\text{-}008\ r^4 + 4.4348e\text{-}006\ r^3 - 0.00017006\ r^2 + 0.00037434\ r + 0.070987;$

$varxi := 3.019e\text{-}11\ r^5 + 4.1477e\text{-}9\ r^4 - 1.953e\text{-}7\ r^3 + 3.3434e\text{-}6\ r^2 - 1.2286e\text{-}5\ r + 0.00018483;$

$radxi := -5.2996e\text{-}008\ r^4 + 6.6105e\text{-}006\ r^3 - 0.00024469\ r^2 + 0.0009596\ r + 0.070159;$

$Y_{H2} := -49.447\ xi^3 + 13.134\ xi^2 - 0.062525\ xi + 0.0001087;$

$Y_{O2} := -406.7\ xi^3 + 106.57\ xi^2 - 8.7691\ xi + 0.2324;$

$Y_{N2} := -0.85614\ xi + 0.76431;$

$Y_{H2O} := 399.64\ xi^3 - 111.56\ xi^2 + 9.3646\ xi + 0.0043736;$

$Y_{OH} := -29272\ \xi^5 + 6219.6\ \xi^4 - 450.36\ \xi^3 + 10.756\ \xi^2 + 0.030193\ xi - 8.1914e\text{-}005;$

$X_{H2} := -804.34\ xi^3 + 134.01\ xi^2 - 0.51923\ xi + 0.00087041;$

$X_{O2} := -483.33\ xi^3 + 109.57\ xi^2 - 8.2519\ xi + 0.20707;$

$X_{N2} := 270.04\ xi^3 - 22.016\ xi^2 - 4.9431\ xi + 0.78267;$

$X_{H2O} := 995.62\ xi^3 - 216.21\ xi^2 + 13.435\ xi + 0.010105;$

$u := -1.0739e\text{-}008\ r^6 + 9.7854e\text{-}009\ r^5 + 3.9476e\text{-}005\ r^4 - 2.1465e\text{-}005\ r^3 - 0.052641\ r^2 + 0.0057941\ r + 29.366;$

elif $axial(m) = \frac{1}{2}$ **then**
$T := 3.8869e6\ \text{xi}^\wedge 3 - 1.2274e6\ \text{xi}^\wedge 2 + 87273\ \text{xi} + 319.09;$
$meanxi := 3.952e\text{-}007\ r^\wedge 3 - 2.794e\text{-}005\ r^\wedge 2 - 0.00052678\ r + 0.052666;$
$varxi := 3.8138e\text{-}009\ r^\wedge 3 - 4.2188e\text{-}007\ r^\wedge 2 + 9.7324e\text{-}006\ r + 0.00013173;$
$radxi := -1.8559e\text{-}8\ r^\wedge 4 + 2.5313e\text{-}6\ r^\wedge 3 - 9.9684e\text{-}5\ r^\wedge 2 + 2.9359e\text{-}5\ r + 0.051429;$
$Y_{H2} := -2280.3\ \text{xi}^\wedge 4 + 187.06\ \text{xi}^\wedge 3 + 6.195\ \text{xi}^\wedge 2 - 0.037275\ \text{xi} + 8.486e\text{-}5;$
$Y_{O2} := -23761\ \text{xi}^\wedge 4 + 2092.7\ \text{xi}^\wedge 3 + 29.725\ \text{xi}^\wedge 2 - 8.3106\ \text{xi} + 0.23172;$
$Y_{N2} := -0.68091\ \text{xi} + 0.76331;$
$Y_{H2O} := -85.238\ \text{xi}^\wedge 2 + 8.9679\ \text{xi} + 0.0073409;$
$Y_{OH} := -3.2081\ \text{xi}^\wedge 2 + 0.19936\ \text{xi} - 0.00065724;$
$X_{H2} := -898.08\ \text{xi}^\wedge 3 + 154.7\ \text{xi}^\wedge 2 - 1.3366\ \text{xi} + 0.0036654;$
$X_{O2} := -15409\ \text{xi}^\wedge 4 + 1027.9\ \text{xi}^\wedge 3 + 69.31\ \text{xi}^\wedge 2 - 8.191\ \text{xi} + 0.20695;$
$X_{N2} := -8.2471\ \text{xi}^\wedge 2 - 4.8879\ \text{xi} + 0.78142;$
$X_{H2O} := 1280.1\ \text{xi}^\wedge 3 - 249.68\ \text{xi}^\wedge 2 + 14.45\ \text{xi} + 0.0085668;$
$u := 5.3018e\text{-}6\ r^\wedge 4 + 1.0872e\text{-}6\ r^\wedge 3 - 0.018738\ r^\wedge 2 - 0.0022486\ r + 20.786;$
elif $axial(m) = \frac{5}{8}$ **then**
$T := -1.2226e{+}006\ \text{xi}^\wedge 2 + 95476\ \text{xi} + 294.56;$
$meanxi := 2.8364e\text{-}007\ r^\wedge 3 - 2.4755e\text{-}005\ r^\wedge 2 - 4.9003e\text{-}006\ r + 0.036211;$
$varxi := 9.2875e\text{-}011\ r^\wedge 4 - 1.0483e\text{-}008\ r^\wedge 3 + 3.1844e\text{-}007\ r^\wedge 2 - 2.1246e\text{-}006\ r$
$\quad + 9.0718e\text{-}005;$
$radxi := -9.3365e\text{-}009\ r^\wedge 4 + 1.3775e\text{-}006\ r^\wedge 3 - 6.355e\text{-}005\ r^\wedge 2 + 0.00032735\ r + 0.034624;$
$Y_{H2} := 122.45\ \text{xi}^\wedge 3 + 3.8221\ \text{xi}^\wedge 2 - 0.028206\ \text{xi} + 9.6694e\text{-}005;$
$Y_{O2} := 1095.9\ \text{xi}^\wedge 3 + 24.426\ \text{xi}^\wedge 2 - 8.3718\ \text{xi} + 0.2323;$
$Y_{N2} := -0.80191\ \text{xi} + 0.76463;$
$Y_{H2O} := -92.35\ \text{xi}^\wedge 2 + 9.9802\ \text{xi} + 0.00021333;$
$Y_{OH} := -212.16\ \text{xi}^\wedge 3 + 9.0479\ \text{xi}^\wedge 2 + 0.018844\ \text{xi} - 0.00017928;$
$X_{H2} := 111.86\ \text{xi}^\wedge 2 - 1.4121\ \text{xi} + 0.0061922;$
$X_{O2} := 89.204\ \text{xi}^\wedge 2 - 8.7498\ \text{xi} + 0.20952;$
$X_{N2} := -20.487\ \text{xi}^\wedge 2 - 4.5543\ \text{xi} + 0.78044;$
$X_{H2O} := -176.55\ \text{xi}^\wedge 2 + 14.437\ \text{xi} + 0.0050337;$
$u := 0.00000355940\ r^4 - 0.00001372890\ r^3 - 0.0130190\ r^2 + 0.00377570\ r + 17.07130$
$\quad + 8.0825\ 10^{-9}\ r^5;$ *#interpolated function* $u_{L=\frac{5}{8}} = 0.5\left(u_{L=\frac{3}{4}} + u_{L=\frac{1}{2}}\right)$

elif $axial(m) = \frac{3}{4}$ **then**
$T := -1.0231e{+}006\ \text{xi}^\wedge 2 + 93295\ \text{xi} + 341.05;$
$meanxi := 8.808e\text{-}008\ r^\wedge 3 - 9.0225e\text{-}006\ r^\wedge 2 - 0.00013071\ r + 0.026975;$
$varxi := 2.7985e\text{-}011\ r^\wedge 4 - 3.2709e\text{-}009\ r^\wedge 3 + 8.6676e\text{-}008\ r^\wedge 2 - 6.3694e\text{-}009\ r$
$\quad + 6.1275e\text{-}005;$
$radxi := 1.181e\text{-}007\ r^\wedge 3 - 9.561e\text{-}006\ r^\wedge 2 - 0.00020455\ r + 0.025334;$
$Y_{H2} := 7.0761\ \text{xi}^\wedge 2 - 0.09567\ \text{xi} + 0.00042952;$
$Y_{O2} := 1919.2\ \text{xi}^\wedge 3 - 28.172\ \text{xi}^\wedge 2 - 7.9379\ \text{xi} + 0.23167;$

Y_{N2} := 1880.2 xi^3 − 99.059 xi^2 + 0.66676 xi + 0.75384;
Y_{H2O} := −3.2076e+005 xi^4 + 15584 xi^3 − 287.98 xi^2 + 10.663 xi + 0.0053646;
Y_{OH} := 2.5471 xi^2 + 0.081919 xi − 0.00042632;
X_{H2} := 1899.9 xi^3 − 8.9038 xi^2 + 0.15088 xi + 0.00028744;
X_{O2} := 69.865 xi^2 − 8.6457 xi + 0.2094;
X_{N2} := −21.371 xi^2 − 4.5424 xi + 0.77419;
X_{H2O} := −4057.3 xi^3 + 53.278 xi^2 + 11.637 xi + 0.021833;
u := 1.6165e-008 *r*^5 + 1.8170e-006 *r*^4 − 2.8545e-005 *r*^3 − 0.0073 *r*^2 + 0.0098 *r* + 13.3566;

elif *axial*(*m*) = 1 **then**
T := −1.053e6 xi^2 + 1.0267e5 xi + 312.56;
meanxi := 5.4332e-8 *r*^3 - 5.2383e-6 *r*^2 - 3.1863e-5 *r* + 0.014193;
varxi := −2.0749e-11 *r*^4 + 2.1528e-9 *r*^3 - 8.0241e-008 *r*^2 + 9.8372e-007 *r* + 2.8062e-005;
radxi := 5.8268e-8 *r*^3 - 4.8694e-6 *r*^2 - 6.0246e-5 *r* + 0.012775 ;
Y_{H2} := 141.22 xi + 0.0046358;
Y_{O2} := 11498 xi^3 − 337.42 xi^2 − 5.0129 xi + 0.22231;
Y_{N2} := −1.2707 xi + 0.76761;
Y_{H2O} := 9.3837 xi + 0.001009;
Y_{OH} := 12.715 xi^2 − 0.14837 xi + 0.00060113;
X_{H2} := −1.2674e+009 xi^5 + 5.9034e+007 xi^4 − 1.0723e+006 xi^3 + 9446.2 xi^2 − 40.099 xi + 0.065642;
X_{O2} := 7.7288 xi + 0.20535;
X_{N2} := 104.24 xi^2 − 7.7024 xi + 0.79603;
X_{H2O} := −160.26 xi^2 + 16.209 xi − 0.0045258;
u := 5.0164e-7 * *r*^4 + 6.7053e-7 *r*^3 − 3.1053e-3 *r*^2 + 5.8504e-4 *r* + 9.5894;

else
print(*Out of range*);
end if

> *meanxi* := *subs*(*r* = 1e3·*r*, *meanxi*); *varxi* := *subs*(*r* = 1e3·*r*, *varxi*); *radxi* := *subs*(*r* = 1e3·*r*, *radxi*); *u* := *subs*(*r* = 1e3·*r*, *u*)

>

>

Unloading Units:-Standard

> $cpmix := add\left(Y_k \cdot cp_k, k \textbf{ in } [H2, O2, N2, H2O]\right); CP := eval\left(cpmix, \mathrm{xi} = \xi_{\max}(m)\right);$

>

Assigning fast chemistry relations for T annd Y_k outside the measured domain.

> $derivT := piecewise\Big(\xi_{\min}(m) \le \xi \textbf{ and } \xi \le \xi_{\max}(m), diff(T, \mathrm{xi}), \mathrm{xi} < \xi_{\min}(m) \textbf{ or } \big(\mathrm{xi} > \xi_{\max}(m) \textbf{ and } \mathrm{xi} < \xi_{st}\big), T1 - T2 + \frac{QH2}{CP} YH2_1, \xi > \xi_{st} \textbf{ and } \mathrm{xi} > \xi_{\max}(m), T1 - T2$

$$- \frac{QH2}{CP} YH2_1 \cdot \xi_{st} \cdot \frac{1}{\xi_{st} - 1} \Big);$$

$$> derivY_{OH} := piecewise\big(\xi_{\min}(m) \le \xi \textbf{ and } \xi \le \xi_{\max}(m), diff(Y_{OH}, \mathrm{xi}), 0\big);$$

$$derivY_{H2} := piecewise\Big(\xi_{\min}(m) \le \xi \textbf{ and } \xi \le \xi_{\max}(m), diff(Y_{H2}, \mathrm{xi}), \mathrm{xi} > \xi_{\max}(m) \textbf{ and } \xi > \xi_{st}, YH2_1 \frac{1}{\xi_{st} - 1}, 0\Big);$$

$$derivY_{O2} := piecewise\Big(\xi_{\min}(m) \le \xi \textbf{ and } \xi \le \xi_{\max}(m), diff(Y_{O2}, \mathrm{xi}), \mathrm{xi} < \xi_{st} \textbf{ and } \big(\xi < \xi_{\min}(m) \textbf{ or } \mathrm{xi} > \xi_{\max}(m)\big), -YO2_2\Big(1 - \frac{1}{\xi_{st}}\Big)\Big);$$

$$derivY_{N2} := piecewise\big(\xi_{\min}(m) \le \xi \textbf{ and } \xi \le \xi_{\max}(m), diff(Y_{N2}, \mathrm{xi}), -YN2_2\big);$$

$$derivY_{H2O} := piecewise\big(\xi_{\min}(m) \le \xi \textbf{ and } \xi \le \xi_{\max}(m), diff(Y_{H2O}, \mathrm{xi}), -YH2O_2 + 1 - (-YN2_2) - derivY_{O2} - derivY_{H2}\big);$$

$>$

$$> \mathrm{T} := \mathrm{piecewise}\Big(\xi_{\min}(m) \le \mathrm{xi} \textbf{ and } \xi \le \xi_{\max}(m), T, \xi < \xi_{\min}(m) \textbf{ or } \big(\mathrm{xi} \le \xi_{st} \textbf{ and } \mathrm{xi} > \xi_{\max}(m)\big), \mathrm{xi} \cdot T1 + (1 - \mathrm{xi}) \cdot T2 + \frac{QH2}{CP} \cdot YH2_1 \cdot \mathrm{xi}, \xi > \xi_{\max}(m) \textbf{ and } \xi > \xi_{st}, \mathrm{xi} \cdot T1 + (1 - \mathrm{xi}) \cdot T2 + \frac{QH2}{CP} \cdot YH2_1 \cdot \xi_{st} \frac{1 - \mathrm{xi}}{1 - \xi_{st}}\Big);$$

$>$

$$> Y_{OH} := piecewise\big(\xi_{\min}(m) \le \xi \textbf{ and } \xi \le \xi_{\max}(m), Y_{OH}, 0\big);$$

$$Y_{O2} := piecewise\Big(\xi_{\min}(m) \le \xi \textbf{ and } \xi \le \xi_{\max}(m), Y_{O2}, \xi_{\max}(m) < \mathrm{xi} \textbf{ and } \mathrm{xi} < \xi_{st}, YO2_2 \frac{(\xi_{st} - \xi)}{\xi_{st}}, \xi < \xi_{\min}(m), YO2_2 \cdot \frac{(\xi_{st} - \xi)}{\xi_{st}}, 0\Big);$$

$$Y_{N2} := piecewise\big(\xi_{\min}(m) \le \xi \textbf{ and } \xi \le \xi_{\max}(m), Y_{N2}, \xi > \xi_{\max}(m) \textbf{ or } \mathrm{xi} < \xi_{\min}(m), YN2_2 \cdot (1 - \mathrm{xi})\big);$$

$$Y_{H2} := piecewise\Big(\xi_{\min}(m) \le \xi \textbf{ and } \xi \le \xi_{\max}(m), Y_{H2}, \mathrm{xi} > \xi_{\max}(m) \textbf{ and } \mathrm{xi} > \xi_{st}, YH2_1 \cdot \frac{(\xi_{st} - \xi)}{\xi_{st} - 1}, 0\Big);$$

$$Y_{H2O} := piecewise\big(\xi_{\min}(m) \le \xi \textbf{ and } \xi \le \xi_{\max}(m), Y_{H2O}, \xi > \xi_{\max}(m) \textbf{ or } \mathrm{xi} < \xi_{\min}(m), YH2O_2 \cdot (1 - \mathrm{xi}) + 1 - Y_{H2} - Y_{N2} - Y_{O2}\big);$$

$>$

```
>

>
>
> for k in [H2, O2, N2, H2O] do p_k := X_k·p0; end do;
> rho := (xi·rho1·T1 + (1 − xi) rho2·T2) / T;
```

Turbulence model $\nu_T = l^2\left|\frac{du}{dr}\right|$. *For a round jet* $l = \alpha\cdot\delta$, and $\delta = 0.085\,x$ *where* alpha = 0.075.

```
> δ := 0.085 x;
  l := 0.075·δ;
  ν_t := l^2 abs(diff(u, r));
> Diffusion := ν_t / Sc_t;
> ξ_rad := radxi;
> ξ_ax := 1.4391e-16 * x^6 − 3.8068e-13 * x^5 + 4.0685e-10 * x^4 − 2.2454e-7 * x^3
        + 0.67753e-4 * x^2 − 0.10874e-1 * x + 0.81169;
> ξ_ax := subs(x = 1e3 x, ξ_ax);
```

Calculate conductivity of mixture lambda(xi)

```
> λ_mix := 0.5 (add(λ_k·X_k, k in [H2, O2, N2, H2O]) + (add(X_k/λ_k, k in [H2, O2, N2, H2O]))^(-1));
>
> for n from 1 to 14 do

    if n > 1 and pos(m, n) = 0 then
  print(Out of range);

   break;
   else
  ξ_av := eval(meanxi, r = pos(m, n)·1e−3);
  ξ_var := eval(varxi, r = pos(m, n)·1e−3);
  pdf := f(ξ_av, ξ_var);
   rhoxifunc := 2 ·rho·Diffusion·(diff(ξ_rad, r)^2 + diff(ξ_ax, x)^2);
  rhoxi := eval(rhoxifunc, {xi = ξ_av, r = pos(m, n)·1e−3, x = axial(m)·L·1e−3});
   condoverdiff := eval(λ_mix / Diffusion, {xi = ξ_av, x = 1e−3· axial(m)·L, r = 1e−3· pos(m, n)});
```

$Iheat := evalf\left(Int\left(\text{rho}\cdot derivT^2\cdot pdf, \text{xi}=0..1\right)\right);$

$\sigma_{HT} := \dfrac{rhoxi}{2\,(rho2\cdot T2)^2}\,\text{condoverdiff}\cdot\text{Iheat};$

if $whattype(Iheat) \neq float$ **or** $\text{abs}(Iheat) > 1\text{e}15$ **then**

$\sigma_{HT} := \dfrac{rhoxi}{2\,(rho2\cdot T2)^2}\cdot condoverdiff\cdot Quadrature\left(\text{rho}\cdot derivT^2\cdot pdf, \text{xi}=0..1, method = romberg, output = value\right);$

end if;

$heatentropy[m, n] := \sigma_{HT};$

for k **in** $[H2, O2, N2, H2O]$ **do** $potXi_k := eval\left(potTp_k\right)$ **end do**;

$\mu_{fu} := eval\left(potXi_{H2}, \text{xi}=\xi_{st}\right); \mu_{ox} := eval\left(potXi_{O2}+potXi_{N2}, \text{xi}=\xi_{st}\right); \mu_{prod} := eval\left(potXi_{N2} + potXi_{H2O}, \text{xi}=\xi_{st}\right);$

if $eval\left(pdf, \text{xi}=\xi_{st}\right) \geq 0$ **then**

$\sigma_{chem} := rhoxi\cdot\dfrac{1}{2\left(1-\xi_{st}\right)}\,\dfrac{\left(\mu_{fu}+r_f\cdot\mu_{ox}-(1+r_f)\mu_{prod}\right)}{eval\left(T, \text{xi}=\xi_{st}\right)}\,eval\left(pdf, \text{xi}=\xi_{st}\right);$

$chementropy[m, n] := \sigma_{chem};$

end if;

$msum := 0;$

for k **in** $[H2, O2, N2, H2O, OH]$ **do**

$massterm := derivY[k]\text{^}2 * pdf / Y[k];$

$Imass := evalf(Int(massterm, \text{xi}=0..1));$

if `or`$(whattype(Imass) \neq float, \text{abs}(Imass) > 0.1\text{e}13)$ **then**

$Imass := 0;$

end if;

$msum := msum + R * Imass / M[k];$

end do;

$\text{sigma}[mass] := (1/2) * rhoxi * msum;$

$massentropy[m, n] := \text{sigma}[mass];$

$print(n);$

end if;

end do;

\>

\> **chementropy**[***m*, 1 ..10**]; $heatentropy[m, 1..10]; massentropy[m, 1..10];$

\> $chementropy[m, 11..n-1]; heatentropy[m, 11..n-1]; massentropy[m, 11..n-1];$

Write data to text files.

\> $C := convert(chementropy[m, 1..14], matrix);$ **if** $m = 1$ **then** $fc := fopen(\text{"curvefitdimchem.txt"}, WRITE);$ **else** $fc := fopen(\text{"curvefitdimchem.txt"},$

```
APPEND); end if; writedata(fc, C); fclose(fc);
> H := convert(heatentropy[m, 1 ..14], matrix);if m = 1then fh := fopen("curvefitdimheat.txt",
WRITE); else fh := fopen("curvefitdimheat.txt", APPEND); end if; writedata(fh, H);
fclose(fh);
> Mass := convert(massentropy[m, 1 ..14], matrix);if m = 1then fh
:= fopen("curvefitdimmass.txt", WRITE); else fh := fopen("curvefitdimmass.txt",
APPEND); end if; writedata(fh, Mass); fclose(fh);
>
```